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CHEMOMETRIC PROCESSING OF TXRF DATA IN THE ANALYSIS OF WATER SAMPLES

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The work is presented: current using of chemometric techniques in analytical chemistry; determination of uncertainty and contribution of matrix effects in it; exploration of interference between fluorescent characteristic peaks in TXRF analysis of water samples; evaluation of metrological characteristics of analysis, based on building the calibration functions.

Chemometric methods of data analysis are accepted to divide on two main groups: observation of data with discrimination or classification; prediction of new values, calibration [1]. In this work we use the second method. Big amount of works is dedicated to analysis of water samples, drinks and food products and etc. by TXRF. In this connection the key goal of the use chemometric methods is evaluation of accuracy that type of obtained results. Exactly at the building of calibration functions there are deviations and fluctuations, which caused by random reasons, what is uncertainty includes. The concept of «uncertainty» is comprehensively explained by Kadiz R. [2]. Matrix effects in TXRF commonly includes the following reasons of appearance: primary radiation penetrates into a specimen and absorbed; characteristic x-rays are emitted; characteristic x-rays can also be absorbed in the sample in going toward the detection system; characteristic x-rays of higher energy may act to enhance the intensity of lower-energy characteristic x-rays. For elimination of different reasons of appearance spoiled factors in the probe, the pure water has been used as an object of analysis.

As a theoretical basis for determination of spectral interferences is the work of Reinhold Klockenkämper and Alex von Bohlen [3]. According to work, the statistical probability of line interference for two elements is 20% and more than eight thousands different interferences are generally possible. For example, Ne-Kα and Ni-Lα (ΔE = 3 eV), Al-Kα and Br-Lα (ΔE = 6 eV), S-Kα and Mo-Lα (ΔE = 15 eV) and As-Kα and Pb-Lα (ΔE = 8 eV). The Kα lines can even be disturbed by Mα lines. Particular examples are the line or peak coincidences of S-Kα and Pb-Mα (ΔE=38eV) and Mg-Kα and Tb-Mα (ΔE=13eV). The processing of analysis data were conducted by methods as multifactorial calibration and projection on latent structures with data of net peaks and expected values of element's concentrations.

Based on chemometric techniques of analysis the spectrometric data, is possible to make an automation of data processing of analysis. The automation of metrological assurance of measurements is a prerequisite to reach large-scale coverage, rapidity and cost-efficiency of analytical measurements [4].

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